Various Virtual-Reactor Challenges

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SLC workshop, Feb 23-24, 2006

There's a lot to address in addition to numerics and MPI.

- **Disclaimer: I wrote this talk between 1:30 and 3:30 yesterday, and I haven't slept much this week.**
  - ⇒ ***Let's begin with low expectations.***
  - ⇒ ***Apologies to the materials group. I worked while you talked.***
  - ⇒ ***It's all Abder's fault.***

- **Virtual Reactor requires a large multi-disciplinary team.**
  - ⇒ ***It is difficult to build an effective team. It takes a while.***
  - ⇒ ***It is really difficult to build an effective multi-disciplinary team.***
  - ⇒ ***It is really really difficult to build an effective multi-disciplinary team that is geographically dispersed.***
  - ⇒ ***Difficulty scales much worse than linear in N_{people} or $N_{disciplines}$.***
  - ⇒ ***Face-to-face meetings are essential, in my opinion. Video conferences can augment but not replace them.***
  - ⇒ ***People-time for communication is essential and must be in the budget.***

There's a lot to address in addition to numerics and MPI.

- **Virtual Reactor requires coupled-physics code.**
  - ⇒ ***Can't just stitch together codes for the different physical phenomena.***
  - ⇒ ***In the tera- and peta- worlds, can't just stitch together "packages" or "modules" written independently for the different phenomena***
    - **Can't copy data from one set of parallel data containers to another**
    - **Can't stand first-order time discretizations (like simplest operator splitting)**
    - **May sometimes want to implicitly solve coupled *sub-operators***
  - ⇒ ***A phenomenon coupled to others may need different numerical methods (compared to un-coupled case).***

- **Virtual Reactor requires V&V of coupled-physics code.**
  - ⇒ ***Incredibly important in nuclear applications.***
  - ⇒ ***V&V of each phenomenon's simulation is essential but very insufficient.***
  - ⇒ ***Coupled-physics analytic solutions (for verification) are difficult.***
  - ⇒ ***Coupled-physics experiments (validation) are difficult and expensive.***
  - ⇒ ***Uncertainty and error estimates are essential (and difficult).***

There's a lot to address in addition to numerics and MPI.

- **It's a long way from dozens to thousands of processors.**
  - ⇒ ***Today's state-of-art reactor-analysis codes are not close to this.***
  - ⇒ ***Some research codes and general-purpose transport codes are.***

- **It's even farther from 1,000 to 100,000.**
  - ⇒ ***Let's not underestimate this!***
  - ⇒ ***It looks like petascale will require 100's of thousands of threads running simultaneously. This is where the hardware is heading.***
  - ⇒ ***Transport solution methods today do not scale to this level.***
    - Sweeps don't.
    - Block-Jacobi takes more iterations as blocks shrink.
    - We're working on it! ☺

One technical point (sorry – couldn't resist): full coupling.

- **Particle transport phase-space is 6-dimensional (3 position, 2 direction, 1 energy) plus time.**
  - ⇒ ***Medium resolution in direction and energy Þ 10^4-10^5 unknowns per spatial point.***
- **In a steady-state or eigenvalue problem:**

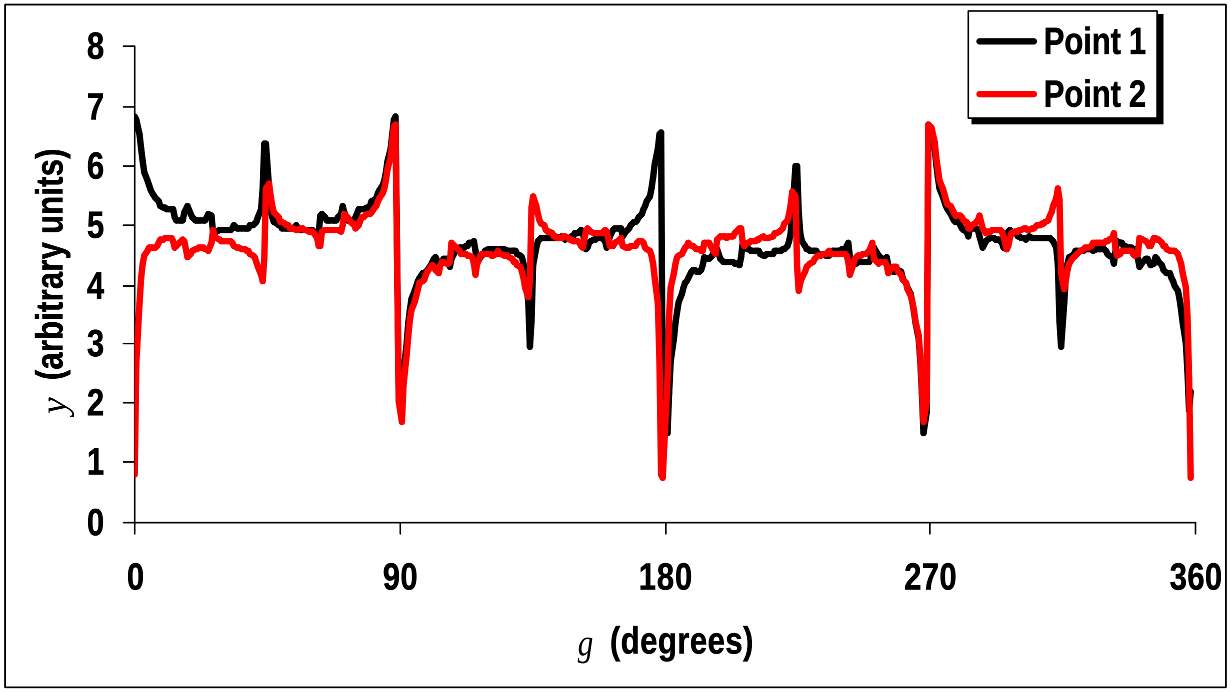
  The solution at each point in phase space influences the solution at every other point in phase space!

  - ⇒ ***Thus, no matter how you decompose the problem, each processor must communicate with every other processor (perhaps indirectly).***
  - ⇒ ***If a transport person collaborates with others on a parallel code, it is very important to convey this point at the beginning!***
- **In a time-dependent problem:**

  The solution at each point in phase space at a given time influences the solution at every other point in phase space at some later time.

Okay, *one more* technical point regarding transport ...

- **When you add resolution in one phase-space variable (for example, resolving true spatial geometry), you complicate the solution in other variables.**
- **Example: explicit fuel pins instead of homogenized pin cells.**



Where we are at Texas A&M

- **At Texas A&M, we have been collaborating closely with math and comp-sci. Team includes:**
  - ⇒ ***Nuclear Engrg*: Marvin Adams, Jim Morel**
  - ⇒ ***Comp-Sci*: Nancy Amato, Lawrence Rauchwerger, Bjarne Stroustrup**
  - ⇒ ***Math*: Raytcho Lazarov, with others coming on board**
- **We have a parallel transport code (PDT). Today it is:**
  - ⇒ ***3D, multigroup, discrete ordinates***
  - ⇒ ***Structured or unstructured (arbitrary polyhedral) grids***
  - ⇒ ***FV and Discontinuous Galerkin spatial discretizations***
  - ⇒ ***TSA preconditioners and Krylov iterative methods (nested)***
  - ⇒ ***Built on solid computer-science infrastructure (STAPL)***
  - ⇒ ***Easy to add new methods – very nice transport testbed!***
- **We are working on:**
  - ⇒ ***A library to support transport calculations***
  - ⇒ ***A multi-physics library / infrastructure***
  - ⇒ ***A nice multi-physics algorithm testbed***
- **Perhaps this is part of a starting point?**